Detailed Procedure of PetaScale Direct Numerical Simulation

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1 Key Equations

1.1 Incompressible Navier-Stokes Equation

The incompressible Navier-Stokes equaion in the tensor notation is

$$\frac{\partial u_i}{\partial t} = -\frac{\partial P}{\partial x_i} + H_i + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \tag{1}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{2}$$

where the nonlinear terms are,

$$H_1 = -\left(\frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} + \frac{\partial uw}{\partial z} \right) \tag{3}$$

$$H_2 = -\left(\frac{\partial uv}{\partial x} + \frac{\partial v^2}{\partial y} + \frac{\partial vw}{\partial z} \right) \tag{4}$$

$$H_3 = -\left(\frac{\partial uw}{\partial x} + \frac{\partial vw}{\partial y} + \frac{\partial w^2}{\partial z} \right) \tag{5}$$

The boundary condition of channel flow is

$$u = v = w = 0 \qquad \text{at} \qquad y = \pm 1 \tag{6}$$

1.2 Pressure

When taking a derivative of by $\partial/\partial x_i$ and summing all directions,

$$\frac{\partial}{\partial t}\left(\frac{\partial u_i}{\partial x_i} \right) = -\frac{\partial^2 P}{\partial x_i \partial x_i} + \frac{\partial H_i}{\partial x_i} + \nu \frac{\partial^2}{\partial x_j \partial x_j}\left(\frac{\partial u_i}{\partial x_i} \right) \tag{7}$$

Due to the continuity, The eq (**??**) becomes,

$$\frac{\partial H_i}{\partial x_i} = \frac{\partial^2 P}{\partial x_i \partial x_i} = \nabla^2 P \tag{8}$$

Hence, the pressure can be calculated by solving the above Poisson equation when the nonlinear terms are calculated.

1.3 g, Vorticity in y-direction

When applying the curl operator to Navier-Stokes equation,

$$\nabla \times \frac{\partial u_i}{\partial t}\mathbf{e}_i = \frac{\partial}{\partial t}\left(\nabla \times u_i \mathbf{e}_i\right) = \frac{\partial}{\partial t}\left(e_{jik}\frac{\partial u_i}{\partial x_j}\mathbf{e}_k\right)$$

$$-\nabla \times \frac{\partial P}{\partial x_i}\mathbf{e}_i = -\nabla \times \nabla P = 0$$

$$\nabla \times H_i \mathbf{e}_i = e_{jik}\frac{\partial H_i}{\partial x_j}\mathbf{e}_k$$

$$\nabla \times \frac{1}{Re}\nabla^2 u_i \mathbf{e}_i = \frac{1}{Re}\nabla^2 e_{jik}\frac{\partial u_i}{\partial x_j}\mathbf{e}_k$$

When $k = 2$, the above equations can be written as,

$$\frac{\partial g}{\partial t} = h_g + \nu \nabla^2 g \tag{9}$$

where,

$$g = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}$$

and,

$$\begin{aligned} h_g &= \frac{\partial H_1}{\partial z} - \frac{\partial H_3}{\partial x} \\ &= -\frac{\partial^2 u^2}{\partial x \partial z} - \frac{\partial^2 uv}{\partial y \partial z} - \frac{\partial^2 uw}{\partial z^2} + \frac{\partial^2 uw}{\partial x^2} + \frac{\partial^2 vw}{\partial x \partial y} + \frac{\partial^2 w^2}{\partial x \partial z} \end{aligned}$$

$$h_g = \frac{\partial^2 (w^2 - u^2)}{\partial x \partial z} - \frac{\partial^2 uv}{\partial y \partial z} - \frac{\partial^2 uw}{\partial z^2} + \frac{\partial^2 uw}{\partial x^2} + \frac{\partial^2 vw}{\partial x \partial y} \tag{10}$$

The boundary condition for g is,

$$g = 0 \qquad at \qquad y = \pm 1 \tag{11}$$

1.4 ϕ

When applying the Laplacian operator to the Navier-Stokes equation of $v(i=2)$,

$$\frac{\partial}{\partial t}\nabla^2 v = -\nabla^2\frac{\partial P}{\partial y} + \nabla^2 H_2 + \nu\nabla^4 v \tag{12}$$

The first two terms of RHS can be re-written as

$$\begin{aligned}
\nabla^2 H_2 - \nabla^2\frac{\partial P}{\partial y} &= \frac{\partial}{\partial y}\left(\frac{\partial}{\partial y}H_2 - \nabla^2 P\right) + \frac{\partial^2 H_2}{\partial x^2} + \frac{\partial^2 H_2}{\partial z^2} && (13)\\
&= \frac{\partial}{\partial y}\left(\frac{\partial H_2}{\partial y} - \frac{\partial H_1}{\partial x} - \frac{\partial H_2}{\partial y} - \frac{\partial H_3}{\partial z}\right) + \frac{\partial^2 H_2}{\partial x^2} + \frac{\partial^2 H_2}{\partial z^2} && (14)\\
&= -\frac{\partial}{\partial y}\left(\frac{\partial H_1}{\partial x} + \frac{\partial H_3}{\partial z}\right) + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)H_2 && (15)
\end{aligned}$$

Hence, Eq (**??**) can be written as,

$$\frac{\partial\phi}{\partial t} = h_v + \nu\nabla^2\phi \tag{16}$$

where,

$$\phi = \nabla^2 v \tag{17}$$

and,

$$\begin{aligned}
h_v =& -\frac{\partial}{\partial y}\left(\frac{\partial H_1}{\partial x} + \frac{\partial H_3}{\partial z}\right) + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)H_2\\
=&\frac{\partial^3 u^2}{\partial x^2\partial y} + \frac{\partial^3 uv}{\partial x\partial y^2} + \frac{\partial^3 uw}{\partial x\partial y\partial z} + \frac{\partial^3 uw}{\partial x\partial y\partial z} + \frac{\partial^3 vw}{\partial y^2\partial z} + \frac{\partial^3 w^2}{\partial y\partial z^2}\\
&-\frac{\partial^3 uv}{\partial x^3} - \frac{\partial^3 v^2}{\partial x^2\partial y} - \frac{\partial^3 vw}{\partial x^2\partial z} - \frac{\partial^3 uv}{\partial x\partial z^2} - \frac{\partial^3 v^2}{\partial y\partial z^2} - \frac{\partial^3 vw}{\partial z^3}
\end{aligned}$$

$$\begin{aligned}
h_v =&\frac{\partial^3(u^2-v^2)}{\partial x^2\partial y} + \frac{\partial^3(w^2-v^2)}{\partial y\partial z^2} + 2\frac{\partial^3 uw}{\partial x\partial y\partial z} + \frac{\partial^3 uv}{\partial x\partial y^2} + \frac{\partial^3 vw}{\partial y^2\partial z}\\
&-\frac{\partial^3 uv}{\partial x^3} - \frac{\partial^3 vw}{\partial x^2\partial z} - \frac{\partial^3 uv}{\partial x\partial z^2} - \frac{\partial^3 vw}{\partial z^3}
\end{aligned}$$

The boundary conditions are,

$$v = \frac{\partial v}{\partial y} = 0, \qquad at \qquad y = \pm 1 \tag{18}$$

1.5 Calculating u,v and w from ϕ and g

The fields are in wavespace which is transformed in x and z directions. In wavespace, Eq(**??**) and (**??**) becomes as

$$g = ik_z u - ik_x w \tag{19}$$

$$\phi = -k_x^2 v + \frac{\partial^2}{\partial y^2} v - k_z^2 v \tag{20}$$

2 Numerical Algorithm

2.1 Low Storage 3rd Order Runge-Kutta scheme

$$\frac{\partial \mathbf{u}}{\partial t} = L(\mathbf{u}) + N(\mathbf{u})$$

where L denotes linear operator and N denotes nonlinear operator.

$$\begin{aligned}
\mathbf{u}' &= \mathbf{u}_n + \Delta t \left[\alpha_0 L\left(\mathbf{u}_n\right) + \beta_0 L\left(\mathbf{u}'\right) + \gamma_0 N\left(\mathbf{u}_n\right)\right] \\
\mathbf{u}'' &= \mathbf{u}' + \Delta t \left[\alpha_1 L\left(\mathbf{u}'\right) + \beta_1 L\left(\mathbf{u}''\right) + \gamma_1 N\left(\mathbf{u}'\right) + \zeta_1 N\left(\mathbf{u}_n\right)\right] \\
\mathbf{u}_{n+1} &= \mathbf{u}'' + \Delta t \left[\alpha_2 L\left(\mathbf{u}''\right) + \beta_2 L\left(\mathbf{u}_{n+1}\right) + \gamma_2 N\left(\mathbf{u}''\right) + \zeta_2 N\left(\mathbf{u}'\right)\right]
\end{aligned}$$

In generally,

$$\mathbf{u}_{i+1} = \mathbf{u}_i + \Delta t \left[\alpha_i L\left(\mathbf{u}_i\right) + \beta_i L\left(\mathbf{u}_{i+1}\right) + \gamma_i N\left(\mathbf{u}_i\right) + \zeta_i N\left(\mathbf{u}_{i-1}\right)\right]$$

$$\mathbf{u}_{i+1} - \beta_i \Delta t L\left(\mathbf{u}_{i+1}\right) = \mathbf{u}_i + \Delta t \alpha_i L\left(\mathbf{u}_i\right) + \Delta t \gamma_i N\left(\mathbf{u}_i\right) + \Delta t \zeta_i N\left(\mathbf{u}_{i-1}\right)$$

where,

$$\begin{array}{cccc}
\alpha_1 = \frac{29}{96} & \beta_1 = \frac{37}{160} & \gamma_1 = \frac{8}{15} & \zeta_1 = 0 \\
\alpha_2 = -\frac{3}{40} & \beta_2 = \frac{5}{24} & \gamma_2 = \frac{5}{12} & \zeta_2 = -\frac{17}{60} \\
\alpha_3 = \frac{1}{6} & \beta_3 = \frac{1}{6} & \gamma_3 = \frac{3}{4} & \zeta_3 = -\frac{5}{12}
\end{array}$$

2.2 Low wavenumber forcing

2.3 Data Structure

2.4 Transpose - Pencil

2.5 Compact Finite Difference

2.5.1 Approximation of the First Derivative

For uniform mesh,

$$\beta f'_{i-2} + \alpha f'_{i-1} + f'_i + \alpha f'_{i+1} + \beta f'_{i+2} = c\frac{f_{i+3} - f_{i-3}}{6h} + b\frac{f_{i+2} - f_{i-2}}{4h} + a\frac{f_{i+1} - f_{i-1}}{2h} \tag{21}$$

At the boundary,

$$f'_1 + \alpha f'_2 = \frac{1}{h}\left(af_1 + bf_2 + cf_3 + df_4\right) \tag{22}$$

Simply, let's denote as

$$A_1\mathbf{f}' = B_1\mathbf{f} \tag{23}$$

2.5.2 Approximation of the Second Derivative

For uniform mesh,

$$\beta f''_{i-2} + \alpha f''_{i-1} + f''_i + \alpha f''_{i+1} + \beta f''_{i+2} = c\frac{f_{i+3} - 2f_i + f_{i-3}}{9h^2} + b\frac{f_{i+2} - 2f_i + f_{i-2}}{4h^2} + a\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \tag{24}$$

At the boundary,

$$f''_1 + \alpha f''_2 = \frac{1}{h^2}\left(af_1 + bf_2 + cf_3 + df_4 + ef_5\right) \tag{25}$$

Simply, let's denote as

$$A_2\mathbf{f}'' = B_2\mathbf{f} \tag{26}$$

2.5.3 Non-Uniform Grid

When g denote the uniform grid, and x denote the non-uniform grid, The following relation can be used to transform uniform mesh to non-uniform grid.

$$\frac{df}{dx} = \frac{dg}{dx}\frac{df}{dg} \tag{27}$$

For the second derivative,

$$\frac{d^2f}{dg^2} = \frac{d}{dg}\left(\frac{df}{dg}\right) = \frac{d}{dg}\left(\frac{df}{dg}\frac{df}{dx}\right) = \frac{df}{dx}\frac{d^2x}{dg^2} + \frac{dx}{dg}\frac{d^2f}{dgdx} = \frac{df}{dx}\frac{d^2x}{dg^2} + \left(\frac{dx}{dg}\right)^2\frac{d^2f}{dx^2}$$

Hence,

$$\frac{d^2f}{dx^2} = \frac{\frac{d^2f}{dg^2} - \frac{df}{dx}\frac{d^2x}{dg^2}}{\left(\frac{dx}{dg}\right)^2} \tag{28}$$

2.6 B-Spline

Let a domain $[-1, 1]$ divided into N intervals with $N+1$ grid points $x_0, x_1, \cdots, x_i, \cdots, x_N$. Also, non-decreasing $N+k$ are determined; $t_0, t_1, \cdots, t_j, \cdots, t_N, t_{N+1}, \cdots, t_{N+k}$. $N+k$ B-splines of order k can be generated by following recursion relationship.

$$B_j^k(x_i) = \frac{x_i - t_{j-k-1}}{t_{j-1} - t_{j-k-1}}B_{j-1}^{k-1}(x_i) + \frac{t_j - x_i}{t_j - t_{j-k}}B_j^{k-1}(x_i), \qquad j = 1, 2, \cdots, N+k$$

When k is zero,

$$B_j^0(x_i) = \begin{cases} 1 & \text{if} \quad t_{j-1} < x_i \leq t_j \\ 0 & \text{otherwise} \end{cases}$$

When the known data $u(x_0), u(x_1), \cdots, u(x_i), \cdots, u(x_N)$ are given, the function can be approximated as the linear combination of B-spline basis functions.

$$u(x_i) \approx U(x_i) = \sum_{j=1}^{N} c_j B_j^k(x_i)$$

From (**??**), mth derivative can be evaluated as,

$$\frac{d^m}{dx_i^m}u(x_i) \approx \sum_{j=1}^{N} c_j \frac{d^m}{dx_i^m}B_j^k(x_i)$$

The mth derivative of the B-spline basis functions are

$$\frac{d^m}{dx_i^m}B_j^k(x_i) = \sum_{l=j-1}^{j} \alpha_{jl}^m B_l^{k-m}(x_i)$$

where the coefficients α are

$$\alpha_{jl}^0 = \delta_{jl}\ , \qquad \alpha_j^{m+1}l = (k-m)\frac{\alpha_{j(l+1)}^m - \alpha_{jl}^m}{t_l - t_{l-k+m}}$$

2.7 Detailed Procedure

2.7.1 Initialization

Memory allocation, Itinializing MPI, FFTW, Coordinate System, etc.

2.7.2 REALSPACE - Nonlinear Product

If RK step is “0”, the maximum velocity is calculated in this step. In this step, non-linear products of velocity component is calculated and stored in U.

2.7.3 HVHG - Calculate h_v and h_g

In this step, the non-linear terms, 'h_v and h_g', which will be used to solve the Poisson eqaution for g and ϕ, is calculated.

$$\begin{aligned} h_v = &-\frac{\partial}{\partial y}\left(k_x^2\left(u^2 - v^2\right)\right) + 2k_xk_zuw + k_z^2(w^2 - v^2)\big) + \frac{\partial^2}{\partial y^2}\left(ik_xuv + ik_zvw\right) \\ &+ ik_x^3\, uv + ik_x^2k_z\, vw + ik_xk_z^2\, uv + ik_z^3 vw \end{aligned}$$

$$h_g = k_xk_z\left(u^2 - w^2\right) - ik_z\frac{\partial uv}{\partial y} + k_z^2\, uw - k_x^2\, uw + ik_x\frac{\partial vw}{\partial y}$$

2.7.4 SOLVE_V_F - solve for v and f

In this step, the following equations are solved for g and ϕ.

$$\frac{\partial g}{\partial t} = h_g + \nu\nabla^2 g \tag{29}$$

$$\frac{\partial \phi}{\partial t} = h_v + \nu\nabla^2 \phi \tag{30}$$

To apply the low storage 3rd order Runge-Kutta algorithm, the Eq (**??**) will be modified as

$$g_{i+1} = g_i + \Delta t\alpha_i\nu\nabla^2 g_i + \Delta t\beta_i\nu\nabla^2 g_{i+1} + \Delta t\gamma_i h_{g,i} + \Delta t\zeta_i h_{g,i-1} \tag{31}$$

$$\left(1 - \Delta t\beta_i\nu\nabla^2\right) g_{i+1} = g_i + \Delta t\alpha_i\nu\nabla^2 g_i + \Delta t\gamma_i h_{g,i} + \Delta t\zeta_i h_{g,i-1} \tag{32}$$

The boundary condtion is

$$g = 0 \qquad at \qquad y = \pm 1$$

Similarly, to apply the low storage 3rd order Runge-Kutta algorithm, the Eq (**??**) will be modified as

$$\left(1-\Delta t\beta_i\nu\nabla^2\right)\phi_{i+1}=\phi_i+\Delta t\alpha_i\nu\nabla^2\phi_i+\Delta t\gamma_i h_{v,i}+\Delta t\zeta_i h_{v,i-1} \tag{33}$$

The boundary condition is

$$v_{i+1}(\pm1)=\frac{\partial v_{i+1}}{\partial y}(\pm1)=0,\qquad \nabla^2 v_{i+1}=\phi_{i+1} \tag{34}$$

To satisfy the four boundary conditions as follows. Let

$$v=v_p+c_1v_{h1}+c_2v_{h2} \tag{35}$$

$$\phi=\phi_p+c_1\phi_{h1}+c_2\phi_{h2} \tag{36}$$

$$\nabla^2 v_{p,i+1}=\phi_{p,i+1},\qquad \nabla^2 v_{h1,i+1}=\phi_{h1,i+1},\qquad \nabla^2 v_{h2,i+1}=\phi_{h2,i+1} \tag{37}$$

where the particular solution $v_{p,i+1}$, and the two homogeneous solutions $v_{h1,i+1}$ and $v_{h2,i+1}$ satisfy following equations.

$$\left(1-\Delta t\beta_i\nu\nabla^2\right)\phi_{p,i+1}=\phi_i+\Delta t\alpha_i\nu\nabla^2\phi_i+\Delta t\gamma_i h_{v,i}+\Delta t\zeta_i h_{v,i-1} \tag{38}$$

$$\phi_{p,i+1}(\pm1)=0,\qquad v_{p,i+1}(\pm1)=0 \tag{39}$$

$$\left(1-\Delta t\beta_i\nu\nabla^2\right)\phi_{h1,i+1}=0 \tag{40}$$

$$\phi_{h1,i+1}(+1)=0,\qquad \phi_{h1,i+1}(-1)=1,\qquad v_{h1,i+1}(\pm1)=0 \tag{41}$$

$$\left(1-\Delta t\beta_i\nu\nabla^2\right)\phi_{h2,i+1}=0 \tag{42}$$

$$\phi_{h2,i+1}(+1)=1,\qquad \phi_{h2,i+1}(-1)=0,\qquad v_{h2,i+1}(\pm1)=0 \tag{43}$$

The constant c_1 and c_2 are chosen such that

$$\frac{\partial v_{i+1}}{\partial y}(\pm1)=0 \tag{44}$$

One can compute the f after the constant c_1 and c_2 are chosen.

$$f = \frac{\partial v}{\partial y} = -\left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z}\right) \tag{45}$$

- Using B-Spline

Let

$$\mathbf{u} \approx B_0 \mathbf{c}_u, \qquad \frac{\partial \mathbf{u}}{\partial y} \approx B_1 \mathbf{c}_u, \qquad \frac{\partial^2 \mathbf{u}}{\partial y^2} \approx B_2 \mathbf{c}_u \tag{46}$$

and

$$\nabla^2 = -k_x^2 - k_z^2 + \frac{\partial^2}{\partial y^2} \tag{47}$$

Then, Eq(**??**), Eq(**??**), Eq(**??**) and Eq(**??**) can be rewritten as

$$\left(\left(1 + \Delta t \beta_i \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_i \nu B_2\right) c_{g,i+1} = \left(1 - \Delta t \alpha_i \nu (k_x^2 + k_z^2)\right) g_i + \Delta t \alpha_i \nu B_2 c_{g,i} + \Delta t \gamma_i h_{g,i} + \Delta t \zeta_i h_{g,i-1} \tag{48}$$

$$\left(\left(1 + \Delta t \beta_i \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_i \nu B_2\right) c_{\phi_p,i+1} = \left(1 - \Delta t \alpha_i \nu (k_x^2 + k_z^2)\right) \phi_i + \Delta t \alpha_i \nu B_2 c_{\phi,i} + \Delta t \gamma_i h_{v,i} + \Delta t \zeta_i h_{v,i-1} \tag{49}$$

$$\left(\left(1 + \Delta t \beta_i \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_i \nu B_2\right) c_{\phi_{h1},i+1} = 0 \tag{50}$$

$$\left(\left(1 + \Delta t \beta_i \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_i \nu B_2\right) c_{\phi_{h2},i+1} = 0 \tag{51}$$

More specifically, using the low storage RK 3 methods,

- 1st step

$$\left(\left(1 + \Delta t \beta_1 \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_1 \nu B_2\right) c_{g,2} = \left(1 - \Delta t \alpha_1 \nu (k_x^2 + k_z^2)\right) g_1 + \Delta t \alpha_1 \nu B_2 c_{g,1} + \Delta t \gamma_1 h_{g,1} \tag{52}$$

$$\left(\left(1 + \Delta t \beta_1 \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_1 \nu B_2\right) c_{\phi_p,2} = \left(1 - \Delta t \alpha_1 \nu (k_x^2 + k_z^2)\right) \phi_1 + \Delta t \alpha_1 \nu B_2 c_{\phi,1} + \Delta t \gamma_1 h_{v,1} \tag{53}$$

$$\left(\left(1 + \Delta t \beta_1 \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_1 \nu B_2\right) c_{\phi_{h1},2} = 0 \tag{54}$$

$$\left(\left(1 + \Delta t \beta_1 \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_1 \nu B_2\right) c_{\phi_{h2},2} = 0 \tag{55}$$

- 2nd step

$$\left(\left(1 + \Delta t \beta_2 \nu (k_x^2 + k_z^2)\right) B_0 - \Delta t \beta_2 \nu B_2\right) c_{g,3} = \left(1 - \Delta t \alpha_2 \nu (k_x^2 + k_z^2)\right) g_2 + \Delta t \alpha_2 \nu B_2 c_{g,2} + \Delta t \gamma_2 h_{g,2} + \Delta t \zeta_2 h_{g,1} \tag{56}$$

$$\left(\left(1+\Delta t\beta_2\nu(k_x^2+k_z^2)\right)B_0-\Delta t\beta_2\nu B_2\right)c_{\phi_p,3}=\left(1-\Delta t\alpha_2\nu(k_x^2+k_z^2)\right)\phi_1+\Delta t\alpha_2\nu B_2 c_{\phi,2}+\Delta t\gamma_2 h_{v,2}+\Delta t\zeta_i h_{v,1} \tag{57}$$

$$\left(\left(1+\Delta t\beta_2\nu(k_x^2+k_z^2)\right)B_0-\Delta t\beta_2\nu B_2\right)c_{\phi_{h1},3}=0 \tag{58}$$

$$\left(\left(1+\Delta t\beta_2\nu(k_x^2+k_z^2)\right)B_0-\Delta t\beta_2\nu B_2\right)c_{\phi_{h2},3}=0 \tag{59}$$

- 3rd step

$$\left(\left(1+\Delta t\beta_3\nu(k_x^2+k_z^2)\right)B_0-\Delta t\beta_3\nu B_2\right)c_{g,new}=\left(1-\Delta t\alpha_3\nu(k_x^2+k_z^2)\right)g_3+\Delta t\alpha_3\nu B_2 c_{g,3}+\Delta t\gamma_3 h_{g,3}+\Delta t\zeta_3 h_{g,2} \tag{60}$$

$$\left(\left(1+\Delta t\beta_3\nu(k_x^2+k_z^2)\right)B_0-\Delta t\beta_3\nu B_2\right)c_{\phi_p,new}=\left(1-\Delta t\alpha_3\nu(k_x^2+k_z^2)\right)\phi_3+\Delta t\alpha_3\nu B_2 c_{\phi,3}+\Delta t\gamma_3 h_{v,3}+\Delta t\zeta_i h_{v,2} \tag{61}$$

$$\left(\left(1+\Delta t\beta_3\nu(k_x^2+k_z^2)\right)B_0-\Delta t\beta_3\nu B_2\right)c_{\phi_{h1},new}=0 \tag{62}$$

$$\left(\left(1+\Delta t\beta_3\nu(k_x^2+k_z^2)\right)B_0-\Delta t\beta_3\nu B_2\right)c_{\phi_{h2},new}=0 \tag{63}$$

2.7.5 SOLVE_U_W - solve for u, and, w

$$f=\frac{\partial v}{\partial y}=-\left(\frac{\partial u}{\partial x}+\frac{\partial w}{\partial z}\right) \tag{64}$$

$$g=\frac{\partial u}{\partial z}-\frac{\partial w}{\partial x}$$

$$\frac{\partial g}{\partial z}-\frac{\partial f}{\partial x}=\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial z^2}\quad\rightarrow\quad ik_z g-ik_x f=-(k_x^2+k_z^2)u\quad\rightarrow\quad u=i\frac{k_x f-k_z g}{k_x^2+k_z^2}$$

$$-\frac{\partial g}{\partial x}-\frac{\partial f}{\partial z}=\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial z^2}\quad\rightarrow\quad -ik_x g-ik_z f=-(k_x^2+k_z^2)w\quad\rightarrow\quad w=i\frac{k_x g+k_z f}{k_x^2+k_z^2}$$

2.7.6 Forcing

After performing Discrete Fourier Transform in x and z direction, zero-zero mode ($k_x=0$, $k_z=0$) is the sum of velocity components in xz plane at each y grid points, and becomes the average quantity after dividing by number of grids in x and z directions.

Since Reynolds number, geometry and viscosity are all fixed, the bulk velocity has to be constant at all times. In this simulation, we set the bulk velocity in stream wise direction as one, $U_{bulk}=1$ and the bulk velocity in span wise direction as zero, $W_{bulk}=0$ by the definition. At zero-zero mode, the velocity in wall normal direction is zero due to continuity at every y grid points.

At zero-zero mode, N-S equation for the velocity component in stream wise direction is

$$\frac{\partial u}{\partial t} = -\frac{\partial P}{\partial x} - \frac{\partial uv}{\partial y} + \nu \frac{\partial^2 u}{\partial y^2} \tag{65}$$

When applying low-storage RK3 method to Eq(**??**),

$$\left(1 - \Delta t \beta_i \nu \frac{\partial^2}{\partial y^2}\right) u_{i+1} = u_i + \Delta t \alpha_i \nu \frac{\partial^2 u_i}{\partial y^2} - \gamma_i \Delta t \frac{\partial u v_i}{\partial y} - \zeta_i \Delta t \frac{\partial u v_{i-1}}{\partial y} - (\gamma_i + \zeta_i) \Delta t \frac{\partial P}{\partial x} \tag{66}$$

When making all velocity components to vector in wall normal direction and using B-Spline,

$$\left(B_0 - \Delta t \beta_i \nu B_2\right) c_{u,i+1} = u_i + \Delta t \alpha_i \nu \frac{\partial^2 u_i}{\partial y^2} - \gamma_i \Delta t \frac{\partial u v_i}{\partial y} - \zeta_i \Delta t \frac{\partial u v_{i-1}}{\partial y} - (\gamma_i + \zeta_i) \Delta t \frac{\partial P}{\partial x} \tag{67}$$

Above equation can be simply expressed as

$$A\mathbf{c} = \mathbf{n} + \mathbf{p} \tag{68}$$

Where A, $\mathbf{c}$, $\mathbf{n}$, and $\mathbf{p}$ are B-spline mass matrix, B-spline coefficient, RHS except for pressure term and pressure term, respectively. To set the constant bulk velocity the following condition has to be satisfied.

$$U_{bulk} = 1 = \frac{1}{2\delta} \int_{-\delta}^{\delta} u_{i+1} dy = \kappa \cdot \mathbf{c} \tag{69}$$

Where the κ is vector to calculate the integration from B-spline coefficient in given domain. Also, we can set $\mathbf{p}$ as following,

$$\mathbf{p} = \phi \psi \tag{70}$$

where $\psi = (1, 1, 1, \cdots, 1, 1)^T$, and ϕ is scalar which needs to be determined. Finally following equation can be derived.

$$\kappa \cdot \mathbf{c} = \kappa \cdot A^{-1}\mathbf{n} + \kappa \cdot A^{-1}\mathbf{p} = \kappa \cdot A^{-1}\mathbf{n} + \kappa \cdot A^{-1}\phi\psi = 1 \tag{71}$$

When rearranging above equation, we can compute ϕ as,

$$\phi = \frac{1 - \kappa \cdot A^{-1}\mathbf{n}}{\kappa \cdot A^{-1}\psi} \tag{72}$$

Since we have ϕ, we can compute new velocity with forcing. In span wise direction everything is same except for $W_{bulk} = 0$.